

# k-Nearest neighbor density estimation on Riemannian Manifolds.

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## Abstract

In this paper, we consider a k-nearest neighbor kernel type estimator when the random variables belong in a Riemannian manifolds. We study asymptotic properties such as the consistency and the asymptotic distribution. A simulation study is also consider to evaluate the performance of the proposal. Finally, to illustrate the potential applications of the proposed estimator, we analyzed two real example where two different manifolds are considered.

*Key words and phrases:* Asymptotic results, Density estimation, Meteorological applications, Nonparametric, Palaeomagnetic data, Riemannian manifolds.

## 1 Introduction

Let  $X_1, \dots, X_n$  be independent and identically distributed random variables taking values in  $\mathbb{R}^d$  and having density function  $f$ . A class of estimators of  $f$  which has been widely studied since the work of Rosenblatt (1956) and Parzen (1962) has the form

$$f_n(x) = \frac{1}{nh^d} \sum_{j=1}^n K\left(\frac{x - X_j}{h}\right),$$

where  $K(u)$  is a bounded density on  $\mathbb{R}^d$  and  $h$  is a sequence of positive number such that  $h \rightarrow 0$  and  $nh^d \rightarrow \infty$  as  $n \rightarrow \infty$ .

If we apply this estimator to data coming from long tailed distributions, with a small enough  $h$  to appropriate for the central part of the distribution, a spurious noise appears in the tails. With a large value of  $h$  for correctly handling the tails, we can not see the details occurring in the main part of the distribution. To overcome these defects, adaptive kernel estimators were introduced. For instance, a conceptually similar estimator of  $f(x)$  was studied by Wagner (1975) who defined a general neighbor density estimators by

$$\hat{f}_n(x) = \frac{1}{nH_n^d(x)} \sum_{j=1}^n K\left(\frac{x - X_j}{H_n(x)}\right),$$

where  $H_n(x)$  is the distance between  $x$  and the  $k$ -nearest neighbor of  $x$  among  $X_1, \dots, X_n$ , and  $k = k_n$  is a sequence of non-random integers such that  $\lim_{n \rightarrow \infty} k_n = \infty$ . Through these adaptive bandwidth, the estimation in the point  $x$  has the guarantee that to be calculated using at least  $k$  points of the sample.

However, in many applications, the variables  $X$  take values on different spaces than  $\mathbb{R}^d$ . Usually these spaces have a more complicated geometry than the Euclidean space and this has to be taken into account in the analysis of the data. For example if we study the distribution of the stars with luminosity in a given range it is naturally to think that the variables belong to a spherical cylinder ( $S^2 \times \mathbb{R}$ ) instead of  $\mathbb{R}^4$ . If we consider a region of the planet  $M$ , then the direction and the velocity of the wind in this region are points in the tangent bundle of  $M$ , that is a manifold of dimension 4. Other examples could be found in image analysis, mechanics, geology and other fields. They include distributions on spheres, Lie groups, among others, see for example Joshi, et.al. (2007), Goh and Vidal (2008). For this reason, it is interesting to study an estimation procedure of the density function that take into account a more complex structure of the variables.

Nonparametric kernel methods for estimating densities of spherical data have been studied by Hall, et. al (1987) and Bai, et. al. (1988). Pelletier (2005) proposed a family of nonparametric estimators for the density function based on kernel weight when the variables are random object valued in a closed Riemannian manifold. The Pelletier's estimators is consistent with the kernel density estimators in the Euclidean case considered by Rosenblatt (1956) and Parzen (1962).

As we comment above, the importance of local adaptive bandwidth is well known in nonparametric statistics and this is even more true with data taking values on complexity space. In this paper, we propose a  $k$ -nearest neighbor method when the data takes values on a Riemannian manifolds. The proposal combine the ideas of smoothing in Euclidean spaces with the estimators introduced in Pelletier (2005).

This paper is organized as follows. Section 2 contains a brief summary of the necessary concepts of Riemannian geometry. In Section 2.1, we introduce a  $k$ -nearest neighbor estimators on Riemannian manifolds. Uniform consistency of the estimators is derived in Section 3.1, while in Section 3.2 the asymptotic distribution is obtained under regular assumptions. Section 4 contains a Monte Carlo study designed to evaluate the proposed estimators. Finally, Section 5 presents two example using real data. Proofs are given in the Appendix.

## 2 Preliminaries and the estimator

Let  $(M, g)$  be a  $d$ -dimensional Riemannian manifold without boundary. We denote by  $d_g$  the distance induced by the metric  $g$ . With  $B_s(p)$  we denote a normal ball with radius  $s$  centered at  $p$ . The injectivity radius of  $(M, g)$  is given by  $\text{inj}_g M = \inf_{p \in M} \sup\{s \in \mathbb{R} > 0 : B_s(p) \text{ is a normal ball}\}$ . Is easy to see that a compact Riemannian manifold has strictly positive injectivity radius. For example, it is not difficult to see that the  $d$ -dimensional

sphere  $S^d$  endowed with the metric induced by the canonical metric  $g_0$  of  $R^{d+1}$  has injectivity radius equal to  $\pi$ . If  $N$  is a proper submanifold of the same dimension than  $(M, g)$ , then  $\text{inj}_{g|_N} N = 0$ . The Euclidean space or the hyperbolic space have infinity injectivity radius. Moreover, a complete and simply connected Riemannian manifold with non positive sectional curvature has also this property.

Throughout this paper, we will assume that  $(M, g)$  is a complete Riemannian manifold, i.e.  $(M, d_g)$  is a complete metric space. Also we will consider that  $\text{inj}_g M$  is strictly positive. This restriction will be clear in the Section 2.1 when we define the estimator. For standard result on differential and Riemannian geometry we refer to the reader to Boothby (1975), Besse (1978), Do Carmo (1988) and Gallot, Hulin and Lafontaine (2004).

Let  $p \in M$ , we denote with  $0_p$  and  $T_p M$  the null tangent vector and the tangent space of  $M$  at  $p$ . Let  $B_s(p)$  be a normal ball centered at  $p$ . Then  $B_s(0_p) = \exp_p^{-1}(B_s(p))$  is an open neighborhood of  $0_p$  in  $T_p M$  and so it has a natural structure of differential manifold. We are going to consider the Riemannian metrics  $g'$  and  $g''$  in  $B_s(0_p)$ , where  $g' = \exp_p^*(g)$  is the pullback of  $g$  by the exponential map and  $g''$  is the canonical metric induced by  $g_p$  in  $B_s(0_p)$ . Let  $w \in B_s(0_p)$ , and  $(\bar{U}, \bar{\psi})$  be a chart of  $B_s(0_p)$  such that  $w \in \bar{U}$ . We note by  $\{\partial/\partial\bar{\psi}_1|_w, \dots, \partial/\partial\bar{\psi}_d|_w\}$  the tangent vectors induced by  $(\bar{U}, \bar{\psi})$ . Consider the matricial function with entries  $(i, j)$  are given by  $g'((\partial/\partial\bar{\psi}_i|_w), (\partial/\partial\bar{\psi}_j|_w))$ . The volumes of the parallelepiped spanned by  $\{(\partial/\partial\bar{\psi}_1|_w), \dots, (\partial/\partial\bar{\psi}_d|_w)\}$  with respect to the metrics  $g'$  and  $g''$  are given by  $|\det g'((\partial/\partial\bar{\psi}_i|_w), (\partial/\partial\bar{\psi}_j|_w))|^{1/2}$  and  $|\det g''((\partial/\partial\bar{\psi}_i|_w), (\partial/\partial\bar{\psi}_j|_w))|^{1/2}$  respectively. The quotient between these two volumes is independent of the selected chart. So, given  $q \in B_s(p)$ , if  $w = \exp_p^{-1}(q) \in B_s(0_p)$  we can define the volume density function,  $\theta_p(q)$ , on  $(M, g)$  as

$$\theta_p(q) = \frac{|\det g'((\partial/\partial\bar{\psi}_i|_w), (\partial/\partial\bar{\psi}_j|_w))|^{1/2}}{|\det g''((\partial/\partial\bar{\psi}_i|_w), (\partial/\partial\bar{\psi}_j|_w))|^{1/2}}$$

for any chart  $(\bar{U}, \bar{\psi})$  of  $B_s(0_p)$  that contains  $w = \exp_p^{-1}(q)$ . For instance, if we consider a normal coordinate system  $(U, \psi)$  induced by an orthonormal basis  $\{v_1, \dots, v_d\}$  of  $T_p M$  then  $\theta_p(q)$  is the function of the volume element  $d\nu_g$  in the local expression with respect to chart  $(U, \psi)$  evaluated at  $q$ , i.e.

$$\theta_p(q) = \left| \det g_q \left( \frac{\partial}{\partial\psi_i} \Big|_q, \frac{\partial}{\partial\psi_j} \Big|_q \right) \right|^{\frac{1}{2}},$$

where  $\frac{\partial}{\partial\psi_i} \Big|_q = D_{\alpha_i(0)} \exp_p(\dot{\alpha}_i(0))$  with  $\alpha_i(t) = \exp_p^{-1}(q) + tv_i$  for  $q \in U$ . Note that the volume density function  $\theta_p(q)$  is not defined for all the pairs  $p$  and  $q$  in  $M$ , but it is if  $d_g(p, q) < \text{inj}_g M$ .

We finish the section showing some examples of the density function:

- i) In the case of  $(\mathbb{R}^d, g_0)$  the density function is  $\theta_p(q) = 1$  for all  $(p, q) \in \mathbb{R}^d \times \mathbb{R}^d$ .
- ii) In the 2-dimensional sphere of radius  $R$ , the volume density is

$$\theta_{p_1}(p_2) = R \frac{|\text{sen}(d_g(p_1, p_2)/R)|}{d_g(p_1, p_2)} \quad \text{if } p_2 \neq p_1, -p_1 \quad \text{and } \theta_{p_1}(p_1) = 1.$$

where  $d_g$  induced is given by

$$d_g(p_1, p_2) = R \arccos\left(\frac{\langle p_1, p_2 \rangle}{R^2}\right).$$

- iii) In the case of the cylinder of radius 1  $\mathcal{C}_1$  endowed with the metric induced by the canonical metric of  $\mathbb{R}^3$ ,  $\theta_{p_1}(p_2) = 1$  for all  $(p_1, p_2) \in \mathcal{C}_1 \times \mathcal{C}_1$ , and the distance induced is given by  $d_g(p_1, p_2) = d_2((r_1, s_1), (r_2, s_2))$  if  $d_2((r_1, s_1), (r_2, s_2)) < \pi$ , where  $d_2$  is the Euclidean distance of  $\mathbb{R}^2$  and  $p_i = (\cos(r_i), \sin(r_i), s_i)$  for  $i = 1, 2$ .

See also, Besse (1978) and Pennec (2006) for a discussion on the volume density function.

## 2.1 The estimator

Consider a probability distribution with a density  $f$  on a  $d$ -dimensional Riemannian manifold  $(M, g)$ . Let  $X_1, \dots, X_n$  be i.i.d random object takes values on  $M$  with density  $f$ . A natural extension of the estimator proposed by Wagner (1975) in the context of a Riemannian manifold is to consider the following estimator

$$\hat{f}_n(p) = \frac{1}{nH_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} K\left(\frac{d_g(p, X_j)}{H_n(p)}\right),$$

where  $K : \mathbb{R} \rightarrow \mathbb{R}$  is a non-negative function with compact support,  $\theta_p(q)$  denotes the volume density function on  $(M, g)$  and  $H_n(p)$  is the distance  $d_g$  between  $p$  and the  $k$ -nearest neighbor of  $p$  among  $X_1, \dots, X_n$ , and  $k = k_n$  is a sequence of non-random integers such that  $\lim_{n \rightarrow \infty} k_n = \infty$ .

As we mention above, the volume density function is not defined for all  $p$  and  $q$ . Therefore, in order to guarantee the well definition of the estimator we consider a modification of the proposed estimator. Using the fact that the kernel  $K$  has compact support, we consider as bandwidth  $\zeta_n(p) = \min\{H_n(p), \text{inj}_g M\}$  instead of  $H_n(p)$ . Thus, the kernel only considers the points  $X_i$  such that  $d_g(X_i, p) \leq \zeta_n(p)$  that are smaller than  $\text{inj}_g M$  and for these points, the volume density function is well defined. Hence, the  $k$ -nearest neighbor kernel type estimator is defined as follows,

$$\hat{f}_n(p) = \frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} K\left(\frac{d_g(p, X_j)}{\zeta_n(p)}\right), \quad (1)$$

where  $\zeta_n(p) = \min\{H_n(p), \text{inj}_g M\}$ .

**Remark 2.1.1.** If  $(M, g)$  is a compact Riemannian manifold and its sectional curvature is not bigger than  $a > 0$ , then we know by the Lemma of Klingenberg (see Gallot, Hulin, Lafontaine (2004)) that  $\text{inj}_g M \geq \min\{\pi/\sqrt{a}, l/2\}$  where  $l$  is the length of the shortest closed geodesic in  $(M, g)$ .

### 3 Asymptotic results

Denote by  $C^\ell(U)$  the set of  $\ell$  times continuously differentiable functions from  $U$  to  $\mathbb{R}$  where  $U$  is an open set of  $M$ . We assume that the measure induced by the probability  $P$  and by  $X$  is absolutely continuous with respect to the Riemannian volume measure  $d\nu_g$ , and we denote by  $f$  its density on  $M$  with respect to  $d\nu_g$ . More precisely, let  $\mathcal{B}(M)$  be the Borel  $\sigma$ -field of  $M$  (the  $\sigma$ -field generated by the class of open sets of  $M$ ). The random variable  $X$  has a probability density function  $f$ , i.e. if  $\chi \in \mathcal{B}(M)$ ,  $P(X^{-1}(\chi)) = \int_\chi f d\nu_g$ .

#### 3.1 Uniform Consistency

We will consider the following set of assumptions in order to derive the strong consistency results of the estimate  $\hat{f}_n(p)$  defined in (1).

*H1.* Let  $M_0$  be a compact set on  $M$  such that:

- i)  $f$  is a bounded function such that  $\inf_{p \in M_0} f(p) = A > 0$ .
- ii)  $\inf_{p, q \in M_0} \theta_p(q) = B > 0$ .

*H2.* For any open set  $U_0$  of  $M_0$  such that  $M_0 \subset U_0$ ,  $f$  is of class  $C^2$  on  $U_0$ .

*H3.* The sequence  $k_n$  is such that  $k_n \rightarrow \infty$ ,  $\frac{k_n}{n} \rightarrow 0$  and  $\frac{k_n}{\log n} \rightarrow \infty$  as  $n \rightarrow \infty$ .

*H4.*  $K : \mathbb{R} \rightarrow \mathbb{R}$  is a bounded nonnegative Lipschitz function of order one, with compact support  $[0, 1]$  satisfying:  $\int_{\mathbb{R}^d} K(\|\mathbf{u}\|) d\mathbf{u} = 1$ ,  $\int_{\mathbb{R}^d} \mathbf{u} K(\|\mathbf{u}\|) d\mathbf{u} = \mathbf{0}$  and  $0 < \int_{\mathbb{R}^d} \|\mathbf{u}\|^2 K(\|\mathbf{u}\|) d\mathbf{u} < \infty$ .

*H5.* The kernel  $K(u)$  verifies  $K(uz) \geq K(z)$  for all  $u \in (0, 1)$ .

**Remark 3.1.1.** The fact that  $\theta_p(p) = 1$  for all  $p \in M$  guarantees that *H1* ii) holds. The assumption *H3* is usual when dealing with nearest neighbor and the assumption *H4* is standard when dealing with kernel estimators.

**Theorem 3.1.2.** Assume that *H1* to *H5* holds, then we have that

$$\sup_{p \in M_0} |\hat{f}_n(p) - f(p)| \xrightarrow{a.s.} 0.$$

#### 3.2 Asymptotic normality

To derive the asymptotic distribution of the regression parameter estimates we will need two additional assumptions. We will denote with  $\mathcal{V}_r$  the Euclidean ball of radius  $r$  centered at the origin and with  $\lambda(\mathcal{V}_r)$  its Lebesgue measure.

*H5.*  $f(p) > 0$ ,  $f \in C^2(V)$  with  $V \subset M$  an open neighborhood of  $M$  and the second derivative of  $f$  is bounded.

H6. The sequence  $k_n$  is such that  $k_n \rightarrow \infty$ ,  $k_n/n \rightarrow 0$  as  $n \rightarrow \infty$  and there exists  $0 \leq \beta < \infty$  such that  $\sqrt{k_n n^{-4/(d+4)}} \rightarrow \beta$  as  $n \rightarrow \infty$ .

H7. The kernel verifies

- i)  $\int K_1(\|\mathbf{u}\|)\|\mathbf{u}\|^2 d\mathbf{u} < \infty$  as  $s \rightarrow \infty$  where  $K_1(\mathbf{u}) = K'(\|\mathbf{u}\|)\|\mathbf{u}\|$ .
- ii)  $\|\mathbf{u}\|^{d+1} K_2(\mathbf{u}) \rightarrow 0$  as  $\|\mathbf{u}\| \rightarrow \infty$  where  $K_2(\mathbf{u}) = K''(\|\mathbf{u}\|)\|\mathbf{u}\|^2 - K_1(\mathbf{u})$

**Remark 3.2.1.** Note that  $\text{div}(K(\|\mathbf{u}\|)\mathbf{u}) = K'(\|\mathbf{u}\|)\|\mathbf{u}\| + d K(\|\mathbf{u}\|)$ , then using the divergence Theorem, we get that  $\int K'(\|\mathbf{u}\|)\|\mathbf{u}\| d\mathbf{u} = \int_{\|\mathbf{u}\|=1} K(\|\mathbf{u}\|)\mathbf{u} \frac{\mathbf{u}}{\|\mathbf{u}\|} d\mathbf{u} - d \int K(\|\mathbf{u}\|) d\mathbf{u}$ . Thus, the fact that  $K$  has compact support in  $[0, 1]$  implies that  $\int K_1(\mathbf{u}) d\mathbf{u} = -d$ .

On the other hand, note that  $\nabla(K(\|\mathbf{u}\|)\|\mathbf{u}\|^2) = K_1(\|\mathbf{u}\|)\mathbf{u} + 2K(\|\mathbf{u}\|)\mathbf{u}$  and by H4 we get that  $\int K_1(\|\mathbf{u}\|)\mathbf{u} d\mathbf{u} = \mathbf{0}$ .

**Theorem 3.2.2.** Assume H4 to H7. Then we have that

$$\sqrt{k_n}(\hat{f}_n(p) - f(p)) \xrightarrow{\mathcal{D}} \mathcal{N}(b(p), \sigma^2(p))$$

with

$$b(p) = \frac{1}{2} \frac{\beta^{\frac{d+4}{d}}}{(f(p)\lambda(\mathcal{V}_1))^{\frac{2}{d}}} \int_{\mathcal{V}_1} K(\|\mathbf{u}\|) u_1^2 d\mathbf{u} \sum_{i=1}^d \frac{\partial f \circ \psi^{-1}}{\partial u_i \partial u_i} \Big|_{u=0}$$

and

$$\sigma^2(p) = \lambda(\mathcal{V}_1) f^2(p) \int_{\mathcal{V}_1} K^2(\|\mathbf{u}\|) d\mathbf{u}$$

where  $\mathbf{u} = (u_1, \dots, u_d)$  and  $(B_h(p), \psi)$  is any normal coordinate system.

In order to derive the asymptotic distribution of  $\hat{f}_n(p)$ , we will study the asymptotic behavior of  $h_n^d / \zeta_n^d(p)$  where  $h_n^d = k_n / (nf(p)\lambda(\mathcal{V}_1))$ . Note that if we consider  $\tilde{f}_n(p) = k_n / (n\zeta_n^d(p)\lambda(\mathcal{V}_1))$ ,  $\tilde{f}_n(p)$  is a consistent estimator of  $f(p)$  (see the proof of Theorem 3.1.2.). The next Theorem states that this estimator is also asymptotically normally distributed as in the Euclidean case.

**Theorem 3.2.3.** Assume H4 to H6, and let  $h_n^d = k_n / (nf(p)\lambda(\mathcal{V}_1))$ . Then we have that

$$\sqrt{k_n} \left( \frac{h_n^d}{\zeta_n^d(p)} - 1 \right) \xrightarrow{\mathcal{D}} N(b_1(p), 1)$$

with

$$b_1(p) = \left( \frac{\beta^{\frac{d+4}{2}}}{f(p)\mu(\mathcal{V}_1)} \right)^{\frac{2}{d}} \left\{ \frac{\tau}{6d+12} + \frac{\int_{\mathcal{V}_1} u_1^2 d\mathbf{u} L_1(p)}{f(p)\mu(\mathcal{V}_1)} \right\}$$

where  $\mathbf{u} = (u_1, \dots, u_d)$ ,  $\tau$  is the scalar curvature of  $(M, g)$ , i.e. the trace of the Ricci tensor,

$$L_1(p) = \sum_{i=1}^d \left( \frac{\partial^2 f \circ \psi^{-1}}{\partial u_i \partial u_i} \Big|_{u=0} + \frac{\partial f \circ \psi^{-1}}{\partial u_i} \Big|_{u=0} \frac{\partial \theta_p \circ \psi^{-1}}{\partial u_i} \Big|_{u=0} \right)$$

and  $(B_h(p), \psi)$  is any normal coordinate system.

## 4 Simulations

This section contains the results of a simulation study designed to evaluate the performance of the estimator defined in the Section 2.1. We consider three models in two different Riemannian manifolds, the sphere and the cylinder endowed with the metric induced by the canonical metric of  $\mathbb{R}^3$ . We performed 1000 replications of independent samples of size  $n = 200$  according to the following models:

**Model 1 (in the sphere):** The random variables  $X_i$  for  $1 \leq i \leq n$  are i.i.d. Von Mises distribution  $VM(\mu, \kappa)$  i.e.

$$f_{\mu, \kappa}(X) = \left(\frac{k}{2}\right)^{1/2} I_{1/2}(\kappa) \exp\{\kappa X^T \mu\},$$

with  $\mu$  is the mean parameter,  $\kappa > 0$  is the concentration parameter and  $I_{1/2}(\kappa) = \left(\frac{\kappa\pi}{2}\right) \sinh(\kappa)$  stands for the modified Bessel function. This model has many important applications, as described in [16] and [19]. We generate a random sample follows a Von Mises distribution with mean  $(0, 0, 1)$  and concentration parameter 3.

**Model 2 (in the sphere):** We simulate i.i.d. random variables  $Z_i$  for  $1 \leq i \leq n$  following a multivariate normal distribution of dimension 3, with mean  $(0, 0, 0)$  and covariance matrix equals to the identity. We define  $X_i = \frac{Z_i}{\|Z_i\|}$  for  $1 \leq i \leq n$ , therefore the variables  $X_i$  follow an uniform distribution in the two dimensional sphere.

**Model 3 (in the cylinder):** We consider random variables  $X_i = (\mathbf{y}_i, t_i)$  taking values in the cylinder  $S^1 \times \mathbb{R}$ . We generated the model proposed by Mardia and Sutton (1978) where,

$$\mathbf{y}_i = (\cos(\theta_i), \sin(\theta_i)) \sim VM((-1, 0), 5)$$

$$t_i | \mathbf{y}_i \sim N(1 + 2\sqrt{5} \cos(\theta_i), 1).$$

Some examples of variables with this distribution can be found in Mardia and Sutton (1978).

In all cases, for smoothing procedure, the kernel was taken as the quadratic kernel  $K(t) = (15/16)(1 - t^2)^2 I(|x| < 1)$ . We have considered a grid of equidistant values of  $k$  between 5 and 150 of length 20.

To study the performance of the estimators of the density function  $f$ , denoted by  $\hat{f}_n$ , we have considered the mean square error (MSE) and the median square error (MedSE), i.e,

$$\text{MSE}(\hat{f}_n) = \frac{1}{n} \sum_{i=1}^n [\hat{f}_n(X_i) - f(X_i)]^2 .$$

$$\text{MedSE}(\hat{f}_n) = \text{median} |\hat{f}_n(X_i) - f(X_i)|^2 .$$

Figure 1 gives the values of the MSE and MedSE of  $\hat{f}_n$  in the sphere model considering different numbers of neighbors, while Figure 2 shows the cylinder model. The simulation study confirms the good behavior of  $k$ -nearest neighbor estimators, under the different models considered. In all cases, the estimators are stable under large numbers of neighbors. However, as expected, the estimators using a small number of neighbors have a poor behavior, because in the neighborhood of each point there is a small number of samples.

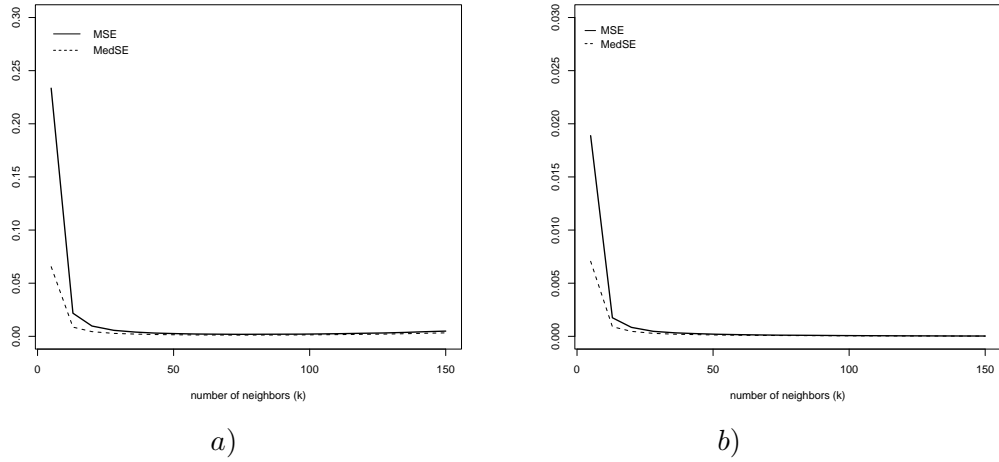


Figure 1: The nonparametric density estimator using different numbers of neighbor, a) the Von Mises model and b) the uniform model.

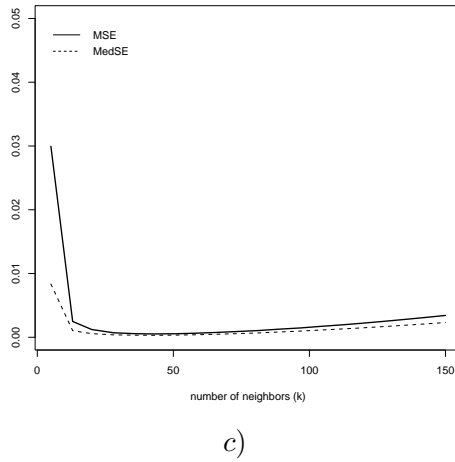


Figure 2: The nonparametric density estimator using different numbers of neighbor in the cylinder.



## 5 Real Example

### 5.1 Paleomagnetic data

It is well known the need for statistical analysis of paleomagnetic data. Since the work developed by Fisher (1953), the study of parametric families was considered a principal tool to analyze and quantify this type of data (see Cox and Doell (1960), Butler (1992) and Love and Constable (2003)). In particular, our proposal allows to explore the nature of directional dataset that include paleomagnetic data without make any parametric assumptions.

In order to illustrate the k-nearest neighbor kernel type estimator on the two-dimensional sphere, we illustrate the estimator using a paleomagnetic data set studied by Fisher, Lewis, and Embleton (1987). The data set consist in  $n = 107$  sites from specimens of Precambrian volcanos with measurements of magnetic remanence. The data set contains two variables corresponding to the directional component on a longitude scale, and the directional component on a latitude scale. The original data set is available in the library `sm` of R statistical package.

To calculate the estimators the volume density function and the geodesic distance were taken as in the Section 2 and we considered the quadratic kernel  $K(t) = (15/16)(1 - t^2)^2 I(|x| < 1)$ . In order to analyze the sensitivity of the results with respect to the number of neighbors, we plot the estimator using different bandwidths. The results are shown in the Figure 3.

The real data was plotted in blue and with a large radius in order to obtain a better visualization. The Equator line, the Greenwich meridian and a second meridian are in gray while the north and south poles are denoted with the capital letter N and S respectively. The levels of concentration of measurements of magnetic remanence can be found in yellow for high levels and in red for lowest density levels. Also, the levels of concentration of measurements of magnetic remanence was illustrated with relief on the sphere that allow to emphasize high density levels and the form of the density function.

As in the Euclidean case large number of neighbors produce estimators with small variance but high bias, while small values produce more wiggly estimators. This fact shows the need of the implementation of a method to select the adequate bandwidth for this estimators. However, this require further careful investigation and are beyond the scope of this paper.

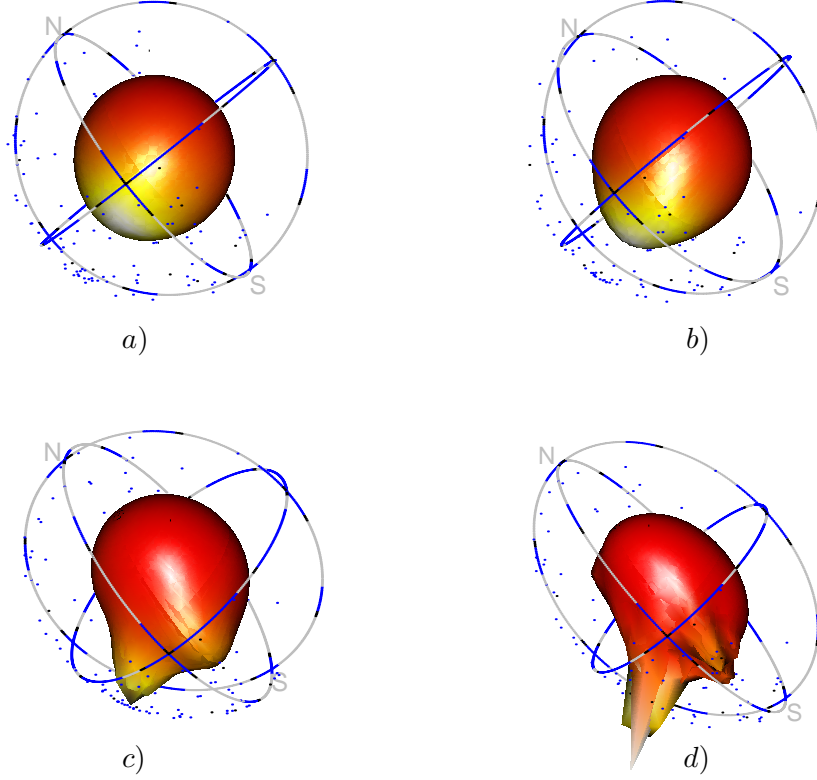


Figure 3: The nonparametric density estimator using different number of neighbors, a)  $k=75$ , b)  $k=50$ , c)  $k=25$  and d)  $k=10$ .

## 5.2 Meteorological data

In this Section, we consider a real data set collected in the meteorological station “Agüita de Perdiz” that is located in Viedma, province of Río Negro, Argentine. The dataset consists in the wind direction and temperature during January 2011 and contains 1326 measurements that were registered with a frequency of thirty minutes. We note that the considered variables belong to a cylinder with radius 1.

As in the previous Section, we consider the quadratic kernel and we took the density function and the geodesic distance as in Section 2. Figure 4 shows the result of the estimators, the color and form of the graphic was constructed as in the previous example.

It is important to remark that the measurement devices of wind direction not present a sufficient precision to avoid repeated data. Therefore, we consider the proposal given in García-Portugués, et.al. (2011) to solve this problem. The proposal consists in perturb the repeated data as follows  $\tilde{r}_i = r_i + \xi \varepsilon_i$ , where  $r_i$  denote the wind direction measurements and  $\varepsilon_i$ , for  $i = 1, \dots, n$  were independently generated from a von Mises distribution with  $\mu = (1, 0)$  and  $\kappa = 1$ . The selection of the perturbation scale  $\xi$  was taken  $\xi = n^{-1/5}$  as in García-Portugués, et.al. (2011) where in this case  $n = 1326$

The work of García-Portugués, et.al. (2011) contains other nice real example where the proposed estimator can be apply. They considered a naive density estimator applied to wind directions and SO2 concentrations, that allow you explore high levels of contamination.

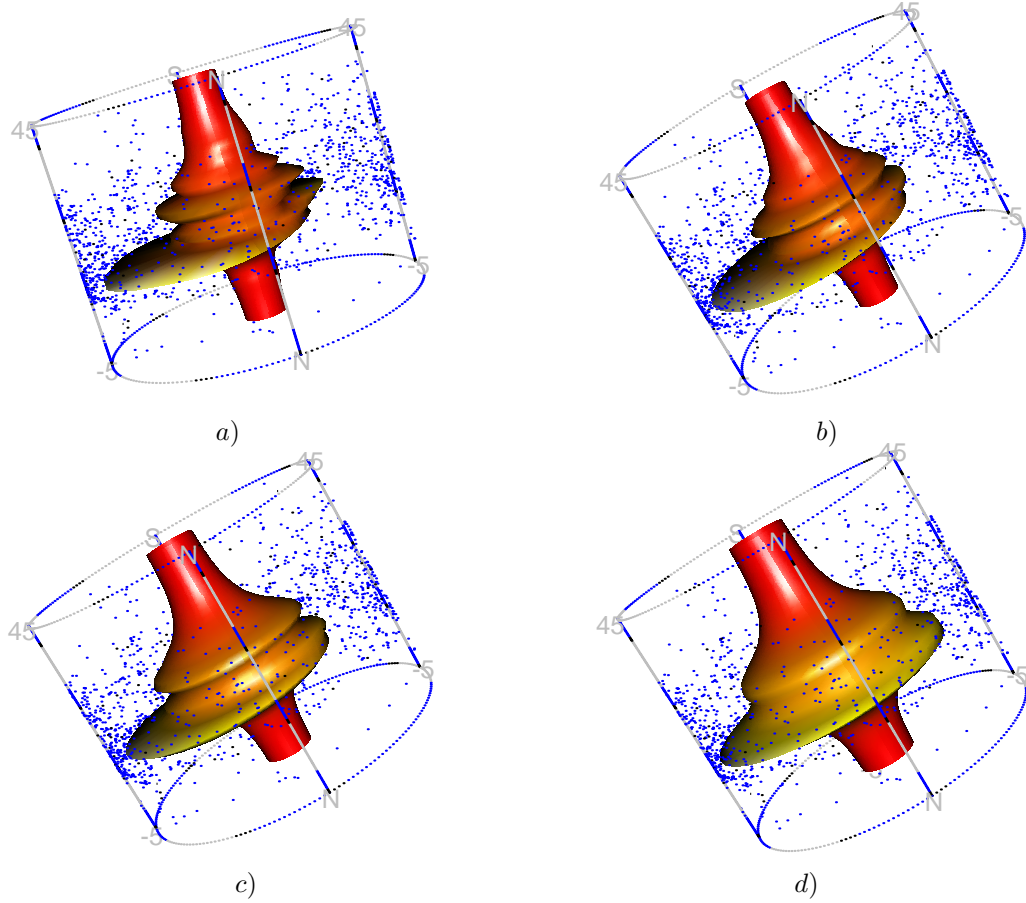


Figure 4: The nonparametric density estimator using different number of neighbors, a)  $k=75$ , b)  $k=150$ , c)  $k=300$  and d)  $k=400$ .

In Figure 4, we can see that the lowest temperature are more probable when the wind comes from the East direction. However, the highest temperature does not seem to have correlation with the wind direction. Also, note that in Figure 4, we can see two mode corresponding to the minimum and maximum daily of the temperature.

These examples show the usefulness of the proposed estimator for the analysis and exploration of these type of dataset.

## Appendix

### Proof of Theorem 3.1.2.

Let

$$f_n(p, \delta_n) = \frac{1}{n\delta_n^d} \sum_{i=1}^n \frac{1}{\theta_{X_i}(p)} K\left(\frac{d_g(p, X_i)}{\delta_n}\right).$$

Note that if  $\delta_n = \delta_n(p)$  verifies  $\delta_{1n} \leq \delta_n(p) \leq \delta_{2n}$  for all  $p \in M_0$  where  $\delta_{1n}$  and  $\delta_{2n}$  satisfy  $\delta_{in} \rightarrow 0$  and  $\frac{n\delta_{in}^d}{\log n} \rightarrow \infty$  as  $n \rightarrow \infty$  for  $i = 1, 2$  then by Theorem 3.2 in Henry and Rodriguez (2009) we have that

$$\sup_{p \in M_0} |f_n(p, \delta_n) - f(p)| \xrightarrow{a.s.} 0 \quad (2)$$

For each  $0 < \beta < 1$  we define,

$$f_n^-(p, \beta) = \frac{1}{nD_n^+(\beta)^d} \sum_{i=1}^n \frac{1}{\theta_{X_i}(p)} K\left(\frac{d_g(p, X_i)}{D_n^-(\beta)}\right) = f_n^-(p, D_n^-(\beta)^d) \frac{D_n^-(\beta)^d}{D_n^+(\beta)^d}.$$

$$f_n^+(p, \beta) = \frac{1}{nD_n^-(\beta)^d} \sum_{i=1}^n \frac{1}{\theta_{X_i}(p)} K\left(\frac{d_g(p, X_i)}{D_n^+(\beta)}\right) = f_n^+(p, D_n^+(\beta)^d) \frac{D_n^+(\beta)^d}{D_n^-(\beta)^d}.$$

where  $D_n^-(\beta) = \beta^{1/2d} h_n$ ,  $D_n^+(\beta) = \beta^{-1/2d} h_n$  and  $h_n^d = k_n / (n\lambda(\mathcal{V}_1)f(p))$  with  $\lambda(\mathcal{V}_1)$  denote the Lebesgue measure of the ball in  $\mathbb{R}^d$  with radius  $r$  centered at the origin. Note that

$$\sup_{p \in M_0} |f_n^-(p, \beta) - \beta f(p)| \xrightarrow{a.s.} 0 \text{ and } \sup_{p \in M_0} |f_n^+(p, \beta) - \beta^{-1} f(p)| \xrightarrow{a.s.} 0. \quad (3)$$

For all  $0 < \beta < 1$  and  $\varepsilon > 0$  we define

$$S_n^-(\beta, \varepsilon) = \{w : \sup_{p \in M_0} |f_n^-(p, \beta) - f(p)| < \varepsilon\},$$

$$S_n^+(\beta, \varepsilon) = \{w : \sup_{p \in M_0} |f_n^+(p, \beta) - f(p)| < \varepsilon\},$$

$$S_n(\varepsilon) = \{w : \sup_{p \in M_0} |\hat{f}_n(p) - f(p)| < \varepsilon\},$$

$$A_n(\beta) = \{f_n^-(p, \beta) \leq \hat{f}_n(p) \leq f_n^+(p, \beta)\}$$

Then,  $A_n(\beta) \cap S_n^-(\beta, \varepsilon) \cap S_n^+(\beta, \varepsilon) \subset S_n(\varepsilon)$ . Let  $A = \sup_{p \in M_0} f(p)$ . For  $0 < \varepsilon < 3A/2$  and  $\beta_\varepsilon = 1 - \frac{\varepsilon}{3A}$  consider the following sets

$$G_n(\varepsilon) = \{w : D_n^-(\beta_\varepsilon) \leq \zeta_n(p) \leq D_n^+(\beta_\varepsilon) \text{ for all } p \in M_0\}$$

$$G_n^-(\varepsilon) = \{\sup_{p \in M_0} |f_n^-(p, \beta_\varepsilon) - \beta_\varepsilon f(p)| < \frac{\varepsilon}{3}\}$$

$$G_n^+(\varepsilon) = \{\sup_{p \in M_0} |f_n^+(p, \beta_\varepsilon) - \beta_\varepsilon^{-1} f(p)| < \frac{\varepsilon}{3}\}.$$

Then we have that  $G_n(\varepsilon) \subset A_n(\beta_\varepsilon)$ ,  $G_n^-(\varepsilon) \subset S_n^-(\beta_\varepsilon, \varepsilon)$  and  $G_n^+(\varepsilon) \subset S_n^+(\beta_\varepsilon, \varepsilon)$ . Therefore,  $G_n(\varepsilon) \cap G_n^-(\varepsilon) \cap G_n^+(\varepsilon) \subset S_n(\varepsilon)$ .

On the other hand, using that  $\lim_{r \rightarrow 0} V(B_r(p))/r^d \mu(\mathcal{V}_1) = 1$ , where  $V(B_r(p))$  denotes the volume of the geodesic ball centered at  $p$  with radius  $r$  (see Gray and Vanhecke (1979)) and similar arguments those considered in Devroye and Wagner (1977), we get that

$$\sup_{p \in M_0} \left| \frac{k_n}{n\lambda(\mathcal{V}_1)f(p)H_n^d(p)} - 1 \right| \xrightarrow{a.s.} 0.$$

Recall that  $\text{inj}_g M > 0$  and  $H_n^d(p) \xrightarrow{a.s.} 0$ . Then for straightforward calculations we obtained that  $\sup_{p \in M_0} \left| \frac{k_n}{n\lambda(\mathcal{V}_1)f(p)\zeta_n^d(p)} - 1 \right| \xrightarrow{a.s.} 0$ . Thus,  $I_{G_n^c(\varepsilon)} \xrightarrow{a.s.} 0$  and (3) imply that  $I_{S_n^c(\varepsilon)} \xrightarrow{a.s.} 0$ .  $\square$

### Proof of Theorem 3.2.2.

A Taylor expansion of second order gives

$$\sqrt{k_n} \left\{ \frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} K \left( \frac{d_g(p, X_j)}{\zeta_n(p)} \right) - f(p) \right\} = A_n + B_n + C_n$$

where

$$\begin{aligned} A_n &= (h_n^d/\zeta_n^d(p))\sqrt{k_n} \left\{ \frac{1}{nh_n^d} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} K \left( \frac{d_g(p, X_j)}{h_n} \right) - f(p) \right\}, \\ B_n &= \sqrt{k_n}((h_n^d/\zeta_n^d(p)) - 1) \left\{ f(p) + \frac{[(h_n/\zeta_n(p)) - 1]h_n^d}{[(h_n^d/\zeta_n^d(p)) - 1]\zeta_n^d(p)} \frac{1}{nh_n^d} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} K_1 \left( \frac{d_g(p, X_j)}{\zeta_n(p)} \right) \right\} \end{aligned}$$

and

$$C_n = \sqrt{k_n}((h_n^d/\zeta_n^d(p)) - 1) \frac{[(h_n/\zeta_n(p)) - 1]^2}{2[(h_n^d/\zeta_n^d(p)) - 1]} \frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} K_2 \left( \frac{d_g(p, X_j)}{\xi_n} \right) [\xi_n/h_n]^2$$

with  $h_n^d = k_n/nf(p)\lambda(\mathcal{V}_1)$  and  $\min(h_n, \zeta_n) \leq \xi_n \leq \max(h_n, \zeta_n)$ . Note that H6 implies that  $h_n$  satisfies the necessary hypothesis given in Theorem 4.1 in Rodriguez and Henry (2009), in particular

$$\sqrt{nh_n^{d+4}} \rightarrow \beta^{\frac{d+4}{d}} (f(p)\lambda(\mathcal{V}_1))^{-\frac{d+4}{2d}}.$$

By the Theorem and the fact that  $h_n/\zeta_n(p) \xrightarrow{p} 1$ , we obtain that  $A_n$  converges to a normal distribution with mean  $b(p)$  and variance  $\sigma^2(p)$ . Therefore it is enough to show that  $B_n$  and  $C_n$  converges to zero in probability.

Note that  $\frac{(h_n/H_n(p))-1}{(h_n^d/\zeta_n^d(p))-1} \xrightarrow{p} d^{-1}$  and by similar arguments those considered in Theorem 3.1 in Pelletier (2005) and Remark 3.2.1. we get that

$$\frac{1}{nh_n^d} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} K_1 \left( \frac{d_g(p, X_j)}{\zeta_n(p)} \right) \xrightarrow{p} \int K_1(\mathbf{u}) d\mathbf{u} f(p) = -d f(p).$$

Therefore, by Theorem 3.2.3., we obtain that  $B_n \xrightarrow{p} 0$ . As  $\xi_n/h_n$  converges to one in probability, in order to concluded the proof, it remains to prove that

$$\frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} |K_2(d_g(p, X_j)/\xi_n)|$$

is bounded in probability.

By H7, there exists  $r > 0$  such that  $|t|^{d+1}|K_2(t)| \leq 1$  if  $|t| \geq r$ . Let  $C_r = (-r, r)$ , then we have that

$$\begin{aligned} \frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} \left| K_2 \left( \frac{d_g(p, X_j)}{\xi_n} \right) \right| &\leq \frac{\sup_{|t| \leq r} |K_2(t)|}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} I_{C_r} \left( \frac{d_g(p, X_j)}{\xi_n} \right) \\ &\quad + \frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} I_{C_r^c} \left( \frac{d_g(p, X_j)}{\xi_n} \right) \left| \frac{d_g(p, X_j)}{\xi_n} \right|^{-(d+1)} \end{aligned}$$

As  $\min(h_n, \zeta_n(p)) \leq \xi_n \leq \max(h_n, \zeta_n(p)) = \tilde{\xi}_n$  it follows that

$$\begin{aligned} \frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} \left| K_2 \left( \frac{d_g(p, X_j)}{\xi_n} \right) \right| &\leq \\ &\leq \left( \frac{h_n}{\zeta_n(p)} \right)^d \sup_{|t| \leq r} |K_2(t)| \frac{1}{nh_n^d} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} I_{C_r} \left( \frac{d_g(p, X_j)}{h_n} \right) \\ &\quad + \sup_{|t| \leq r} |K_2(t)| \frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} I_{C_r} \left( \frac{d_g(p, X_j)}{\zeta_n(p)} \right) \\ &\quad + \left( \frac{h_n}{\zeta_n(p)} \right)^d \frac{1}{nh_n^d} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} I_{C_r^c} \left( \frac{d_g(p, X_j)}{h_n} \right) \left| \frac{d_g(p, X_j)}{h_n} \right|^{-(d+1)} \left| \frac{\tilde{\xi}_n}{h_n} \right|^{(d+1)} \\ &\quad + \frac{1}{n\zeta_n^d(p)} \sum_{j=1}^n \frac{1}{\theta_{X_j}(p)} I_{C_r^c} \left( \frac{d_g(p, X_j)}{\zeta_n(p)} \right) \left| \frac{d_g(p, X_j)}{\zeta_n(p)} \right|^{-(d+1)} \left| \frac{\tilde{\xi}_n}{\zeta_n(p)} \right|^{(d+1)} \\ &= C_{n1} + C_{n2} + C_{n3} + C_{n4}. \end{aligned}$$

By similar arguments those considered in Theorem 3.1 in Pelletier (2005), we have that  $C_{n1} \xrightarrow{p} f(p) \int I_{C_r}(s) ds$  and  $C_{n3} \xrightarrow{p} f(p) \int I_{C_r^c}(s) |s|^{-(d+1)} ds$ .

Finally, let  $A_n^\varepsilon = \{(1 - \varepsilon)h_n \leq \zeta_n \leq (1 + \varepsilon)h_n\}$  for  $0 \leq \varepsilon \leq 1$ . Then for  $n$  large enough  $P(A_n^\varepsilon) > 1 - \varepsilon$  and in  $A_n^\varepsilon$  we have that

$$\begin{aligned} I_{C_r} \left( \frac{d_g(X_j, p)}{\zeta_n(p)} \right) &\leq I_{C_r} \left( \frac{d_g(X_j, p)}{(1 + \varepsilon)h_n} \right), \\ I_{C_r^c} \left( \frac{d_g(X_j, p)}{\zeta_n(p)} \right) \left| \frac{d_g(X_j, p)}{\zeta_n(p)} \right|^{-(d+1)} &\leq I_{C_r^c} \left( \frac{d_g(X_j, p)}{(1 - \varepsilon)h_n} \right) \left| \frac{d_g(X_j, p)}{(1 - \varepsilon)h_n} \right|^{-(d+1)} \left| \frac{\zeta_n(p)}{(1 - \varepsilon)h_n} \right|^{(d+1)}. \end{aligned}$$

This fact and analogous arguments those considered in Theorem 3.1 in Pelletier (2005), allow to conclude the proof.  $\square$

### Proof of Theorem 3.2.3.

Denote  $b_n = h_n^d / (1 + zk_n^{-1/2})$ , then

$$P(\sqrt{k_n}(h_n^d/\zeta_n^d - 1) \leq z) = P(\zeta_n^d \geq b_n) = P(H_n^d \geq b_n, \text{inj}_g M^d \geq b_n).$$

As  $b_n \rightarrow 0$  and  $\text{inj}_g M > 0$ , there exists  $n_0$  such that for all  $n \geq n_0$  we have that

$$P(H_n^d \geq b_n, \text{inj}_g M^d \geq b_n) = P(H_n^d \geq b_n).$$

Let  $Z_i$  such that  $Z_i = 1$  when  $d_g(p, X_i) \leq b_n^{1/d}$  and  $Z_i = 0$  elsewhere. Thus, we have that  $P(H_n^d \geq b_n) = P(\sum_{i=1}^n Z_i \leq k_n)$ . Let  $q_n = P(d_g(p, X_i) \leq b_n^{1/d})$ . Note that  $q_n \rightarrow 0$  and  $nq_n \rightarrow \infty$  as  $n \rightarrow \infty$ , therefore

$$P\left(\sum_{i=1}^n Z_i \leq k_n\right) = P\left(\frac{1}{\sqrt{nq_n}} \sum_{i=1}^n (Z_i - E(Z_i)) \leq \frac{1}{\sqrt{nq_n}}(k_n - nq_n)\right).$$

Using the Lindeberg Central Limit Theorem we easily obtain that  $(nq_n)^{-1/2} \sum_{i=1}^n (Z_i - E(Z_i))$  is asymptotically normal with mean zero and variance one. Hence, it is enough to show that  $(nq_n)^{-1/2}(k_n - nq_n) \xrightarrow{P} z + b_1(p)$ .

Denote by  $\mu_n = n \int_{B_{b_n^{1/d}}(p)} (f(q) - f(p)) d\nu_g(q)$ . Note that  $\mu_n = n q_n - w_n$  with  $w_n = n f(p) V(B_{b_n^{1/d}}(p))$ . Thus,

$$\frac{1}{\sqrt{nq_n}}(k_n - nq_n) = w_n^{-1/2}(k_n - w_n) \left(\frac{w_n}{w_n + \mu_n}\right)^{1/2} + \frac{\mu_n}{w_n^{1/2}} \left(\frac{w_n}{w_n + \mu_n}\right)^{1/2}.$$

Let  $(B_{b_n^{1/d}}(p), \psi)$  be a coordinate normal system. Then, we note that

$$\frac{1}{\lambda(\mathcal{V}_{b_n^{1/d}})} \int_{B_{b_n^{1/d}}(p)} f(q) d\nu_g(q) = \frac{1}{\lambda(\mathcal{V}_{b_n^{1/d}})} \int_{\mathcal{V}_{b_n^{1/d}}} f \circ \psi^{-1}(\mathbf{u}) \theta_p \circ \psi^{-1}(\mathbf{u}) d\mathbf{u}.$$

The Lebesgue's Differentiation Theorem and the fact that  $\frac{V(B_{b_n^{1/d}}(p))}{\lambda(\mathcal{V}_{b_n^{1/d}})} \rightarrow 1$  imply that  $\frac{\lambda_n}{w_n} \rightarrow 0$ . On the other hand, from Gray and Vanhecke (1979), we have that

$$V(B_r(p)) = r^d \lambda(\mathcal{V}_1) (1 - \frac{\tau}{6d+12} r^2 + O(r^4)).$$

Hence, we obtain that

$$\begin{aligned} w_n^{-1/2}(k_n - w_n) &= \frac{w_n^{-1/2} k_n z k_n^{-1/2}}{1 + z k_n^{-1/2}} + \frac{w_n^{-1/2} \tau b_n^{2/d} k_n}{(6d+12)(1 + z k_n^{-1/2})} + w_n^{-1/2} k_n O(b_n^{4/d}) \\ &= A_n + B_n + C_n. \end{aligned}$$

It's easy to see that  $A_n \rightarrow z$  and  $w_n^{-1/2} b_n^{2/d} k_n = \frac{k_n n^{-1/2} b_n^{2/d-1/2}}{(f(p)\lambda(\mathcal{V}_1))^{-2/d}} \left(\frac{b_n \lambda(\mathcal{V}_1)}{V(B_{b_n^{1/d}}(p))}\right)^{1/2}$ , since H6 we obtain that  $B_n \rightarrow \tau \beta^{(d+4)/d} / (6d+12) (f(p)\mu(\mathcal{V}_1))^{-2/d}$ . A similar argument shows that  $C_n \rightarrow 0$  and therefore we get that  $w_n^{-1/2}(k_n - w_n) \rightarrow z + \beta^{\frac{d+4}{d}} \frac{\tau}{6d+12} (f(p)\lambda(\mathcal{V}_1))^{-d/2}$ .

In order to concluded the proof we will show that  $\frac{\mu_n}{w_n^{1/2}} \rightarrow \frac{\beta^{\frac{d+4}{d}}}{(f(p)\lambda(\mathcal{V}_1))^{(d+2)/d}} \int_{\mathcal{V}_1} u_1^2 d\mathbf{u} L_1(p)$ . We use a second Taylor expansion that leads to,

$$\begin{aligned} \int_{B_{b_n^{1/d}}(p)} (f(q) - f(p)) d\nu_g(q) &= \sum_{i=1}^d \frac{\partial f \circ \psi^{-1}}{\partial u_i} \Big|_{u=0} b_n^{1+1/d} \int_{\mathcal{V}_1} u_i \theta_p \circ \psi^{-1}(b_n^{1/d} \mathbf{u}) d\mathbf{u} \\ &+ \sum_{i,j=1}^d \frac{\partial^2 f \circ \psi^{-1}}{\partial u_i \partial u_j} \Big|_{u=0} b_n^{1+2/d} \int_{\mathcal{V}_1} u_i u_j \theta_p \circ \psi^{-1}(b_n^{1/d} \mathbf{u}) d\mathbf{u} \\ &+ O(b_n^{1+3/d}). \end{aligned}$$

Using again a Taylor expansion on  $\theta_p \circ \psi^{-1}(\cdot)$  at 0 we have that

$$\int_{B_{b_n^{1/d}}(p)} (f(q) - f(p)) d\nu_g(q) = b_n^{1+2/d} \int_{\mathcal{V}_1} u_1^2 d\mathbf{u} L_1(p) + O(b_n^{1+3/d})$$

and by  $H6$  the theorem follows.  $\square$

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